



The perks of agent-based modelling with iDynoMiCS 2

Cockx, Bastiaan; Clegg, Robert J.; Lang, Stefan; Smets, Barth F.; Kreft, JanUlrich

Publication date:
2016

Document Version
Publisher's PDF, also known as Version of record

[Link back to DTU Orbit](#)

Citation (APA):
Cockx, B., Clegg, R. J., Lang, S., Smets, B. F., & Kreft, JU. (2016). *The perks of agent-based modelling with iDynoMiCS 2*. Poster session presented at MEWE and biofilms IWA specialist conference, Copenhagen, Denmark.

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

The perks of agent-based modelling with iDynoMiCS 2

Bastiaan J R Cockx¹ (baco@env.dtu.dk), Robert J Clegg², Stefan Lang³, Barth F Smets¹, Jan-Ulrich Kreft²

¹Department of Environmental Engineering, Technical University of Denmark, Bygningstorvet 115, 2800 Kgs. Lyngby, Denmark. ²Centre for Computational Biology, Institute of Microbiology and Infection, School of Biosciences; University of Birmingham, Edgbaston, Birmingham B12 5TT, United Kingdom. ³Department of Bioinformatics, Friedrich Schiller University, Ernst-Abbe-Platz 2, 07743 Jena, Germany



What can we do with an ABM?

Agent based model (ABM) system behavior emerges from the collective behavior of the individually modelled microbial cells. An ABM can capture the effects of a dynamic environment, local interactions, trait variability and adaptation. The approach has proven particularly useful to study spatial explicit problems and/or stochastic systems such as biofilms.

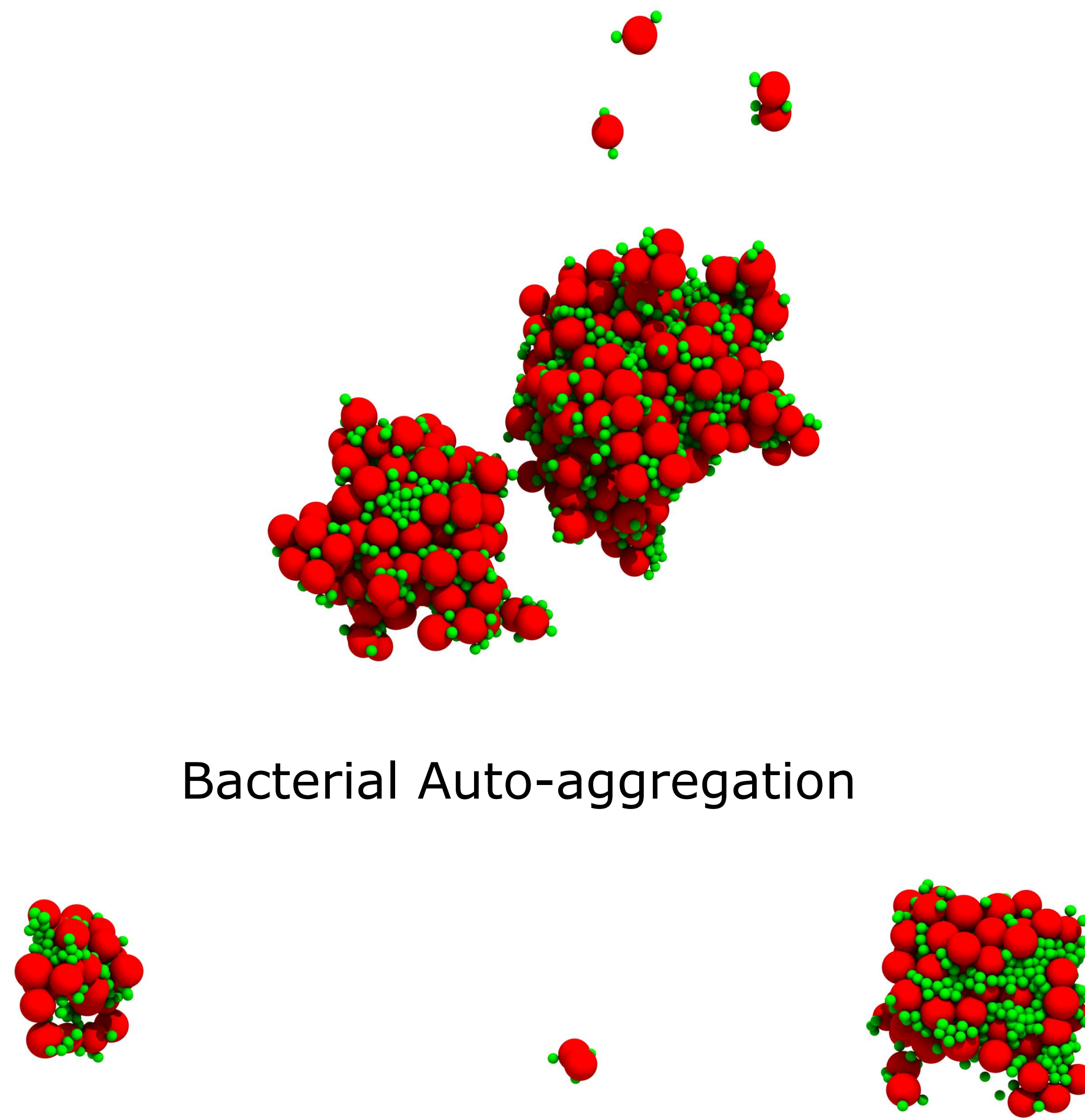
How does an ABM work?

The basic principles and methodology of microbial agent-based models are generally very similar:

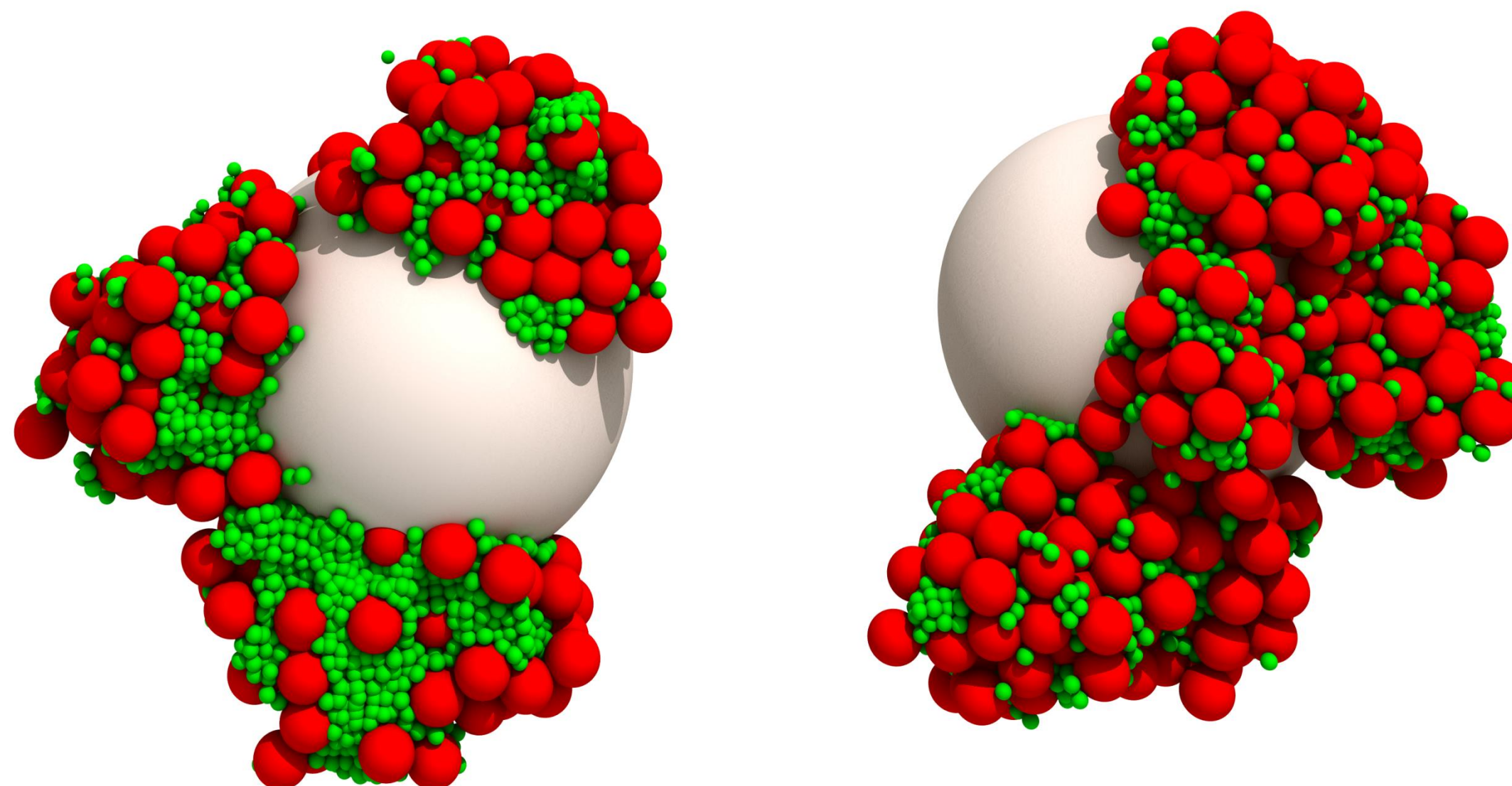
- Agents are represented as discrete entities. Agent behavior is determined by a predefined set of rules. Agents can interact with their local environment by converting solutes, attracting or repelling neighboring agents or by attaching to surfaces.
- The computational domain is discretized and so are all environmental gradients such as solute concentration, pH and temperature. These gradients may change over time due to diffusive or convective transport with neighboring grid cells as well as spontaneous reactions or reactions catalyzed by agents.

The structure and composition of the modelled microbial communities is not programmed, yet it emerges from the chemical and physical interactions of the agents with their environment. This allows us to study the effect of individual agent properties on the development and behavior of the community.

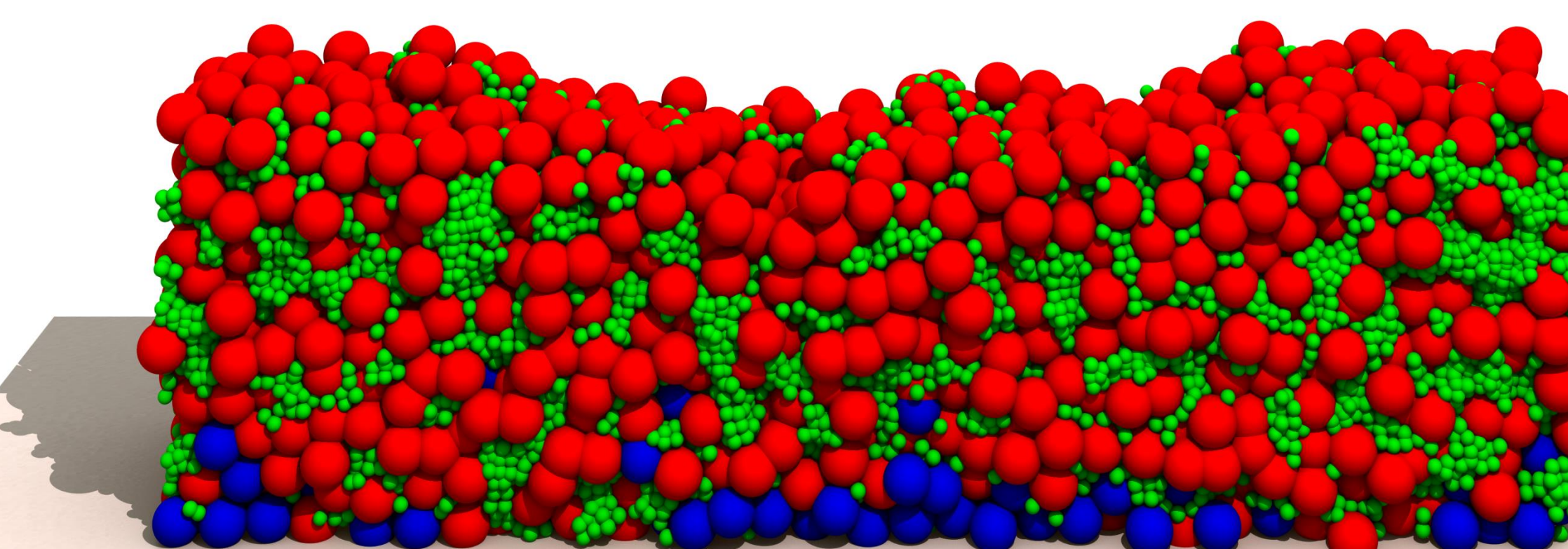
Bacterial Auto-aggregation



Biofilm on carriers



Biofilm on planar surface



iDynoMiCS 2 can be used to study various microbial community types. Aerobic microbe (red), oxygen inhibited microbe (blue), eps (green), carrier surface (gray).

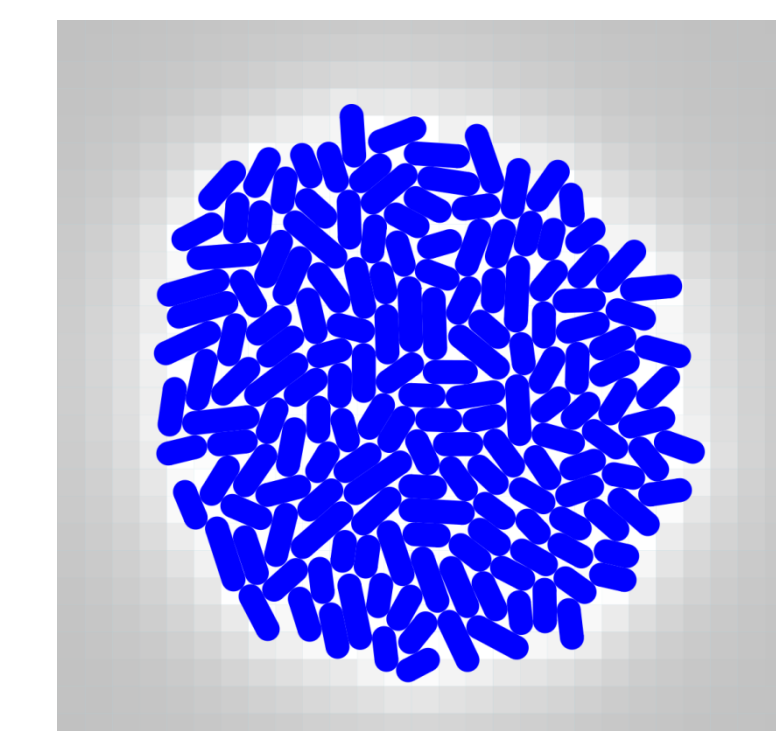
What is iDynoMiCS?

The individual-based Dynamics of Microbial Communities Simulator (iDynoMiCS) is a collective effort to create an extensive multi-purpose ABM framework. The framework provides a common modelling basis, which allows for easy extension for individual research purposes.

What is new in iDynoMiCS 2?

iDynoMiCS 2 provides numerous improvements over the previous version including:

- A modular agent setup allowing for reuse and combination of premade modules including support for non-spherical agent morphology starting with rod-like agents.



iDynoMiCS 2 supports rod-like agent morphology

- Dynamic physical interaction (attraction, repulsion, attachment).
- Spontaneous reactions and Non-Steady-State Diffusion.
- The implementation of non-cubical domains allowing the simulation of cylindrical (pipes, hollow fibers) or spherical (e.g. particulate carrier) model systems.
- Flexible grid sizing and asynchronous solver timing, allowing balancing of model fineness and computational speed.

Take home

- In agent-based models the structure and composition of the modelled microbial community emerges from the behavior and properties of the individual.
- iDynoMiCS 2 is a multi-purpose agent based modelling tool, which is easy to extend for individual research purposes.
- The iDynoMiCS 2 framework is free and open-source. It will be available online (www.idynomics.org) later this year.

Acknowledgement:

This research is supported by the Integrated Water Technology (InWaTech) project, which promotes collaborative research between DTU and KAIST.